

CLAIMS

1. An interaction site prediction apparatus comprising:
 - an input unit that inputs primary sequence information on a target protein;
 - 5 a fragment structure prediction program execution unit that allows a fragment structure prediction program for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input unit;
 - 10 a prediction result comparison unit that compares a fragment structure prediction result of the fragment structure prediction program allowed to execute by the fragment structure prediction program execution unit with the fragment structure prediction result of the other fragment structure prediction program;
 - 15 a frustration calculation unit that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison unit; and
 - an interaction site prediction unit that predicts an interaction site
 - 20 in the target protein based on the frustration of the local part calculated by the frustration calculation unit.
2. An interaction site prediction apparatus comprising:
 - an input unit that inputs primary sequence information on a
 - 25 target protein;

a tertiary structure data acquisition unit that acquires tertiary structure data on the target protein;

a fragment structure prediction program execution unit that allows a fragment structure prediction program for predicting a fragment
5 structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input unit;

a prediction result comparison unit that compares a fragment structure prediction result of the fragment structure prediction program
10 allowed to execute by the fragment structure prediction program execution unit with the tertiary structure data acquired by the tertiary structure data acquisition unit;

a frustration calculation unit that calculates a frustration of a local part of the primary sequence information on the target protein
15 based on a comparison result of the prediction result comparison unit;
and

an interaction site prediction unit that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation unit.

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3. The interaction site prediction apparatus according to claim 1 or 2, further comprising:

a certainty factor information setting unit that sets certainty factor information indicating a certainty factor for the fragment structure
25 prediction result of the fragment structure prediction program, wherein

the frustration calculation unit calculates the frustration of the local part based on the certainty factor information set by the certainty factor information setting unit and on the comparison result.

- 5 4. An interaction site prediction method comprising:
 - an input step that inputs primary sequence information on a target protein;
 - a fragment structure prediction program execution step that allows a fragment structure prediction program for predicting a fragment
 10 structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step;
 - a prediction result comparison step that compares a fragment structure prediction result of the fragment structure prediction program
 15 allowed to execute by the fragment structure prediction program execution step with the fragment structure prediction result of the other fragment structure prediction program;
 - a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein
 20 based on a comparison result of the prediction result comparison step; and
 - an interaction site prediction step that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

5. An interaction site prediction method comprising:

an input step that inputs primary sequence information on a target protein;

5 a tertiary structure data acquisition step that acquires tertiary structure data on the target protein;

a fragment structure prediction program execution step that allows a fragment structure prediction program for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation
10 to the primary sequence information input by the input step;

a prediction result comparison step that compares a fragment structure prediction result of the fragment structure prediction program allowed to execute by the fragment structure prediction program execution step with the tertiary structure data acquired by the tertiary
15 structure data acquisition step;

a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison step;
and

20 an interaction site prediction step that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

6. The interaction site prediction method according to claim 4 or 5,
25 further comprising:

a certainty factor information setting step that sets certainty factor information indicating a certainty factor for the fragment structure prediction result of the fragment structure prediction program, wherein the frustration calculation step calculates the frustration of the local part based on the certainty factor information set by the certainty factor information setting step and on the comparison result.

7. A computer program that makes a computer to execute an interaction site prediction method comprising:

10 an input step that inputs primary sequence information on a target protein;

a fragment structure prediction program execution step that allows a fragment structure prediction program for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step;

15 a prediction result comparison step that compares a fragment structure prediction result of the fragment structure prediction program allowed to execute by the fragment structure prediction program execution step with the fragment structure prediction result of the other fragment structure prediction program;

a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison step;

25 and

an interaction site prediction step that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

- 5 8. A computer program that makes a computer to execute an interaction site prediction method comprising:

an input step that inputs primary sequence information on a target protein;

- 10 a tertiary structure data acquisition step that acquires tertiary structure data on the target protein;

- 15 a fragment structure prediction program execution step that allows a fragment structure prediction program for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step;

- 20 a prediction result comparison step that compares a fragment structure prediction result of the fragment structure prediction program allowed to execute by the fragment structure prediction program execution step with the tertiary structure data acquired by the tertiary structure data acquisition step;

a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison step; and

- 25 an interaction site prediction step that predicts an interaction

site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

9. The program comprising according to claim 7 or 8, further
5 comprising:

a certainty factor information setting step that sets certainty factor information indicating a certainty factor for the fragment structure prediction result of the fragment structure prediction program, wherein
the frustration calculation step calculates the frustration of the
10 local part based on the certainty factor information set by the certainty factor information setting step and on the comparison result.

10. A computer readable recording medium storing a computer program that makes a computer to execute an interaction site prediction
15 method comprising:

an input step that inputs primary sequence information on a target protein;

a fragment structure prediction program execution step that allows a fragment structure prediction program for predicting a fragment
20 structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step;

a prediction result comparison step that compares a fragment structure prediction result of the fragment structure prediction program
25 allowed to execute by the fragment structure prediction program

execution step with the fragment structure prediction result of the other fragment structure prediction program;

a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein
5 based on a comparison result of the prediction result comparison step;
and

an interaction site prediction step that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

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11. A computer readable recording medium storing a computer program that makes a computer to execute an interaction site prediction method comprising:

an input step that inputs primary sequence information on a
15 target protein;

a tertiary structure data acquisition step that acquires tertiary structure data on the target protein;

a fragment structure prediction program execution step that allows a fragment structure prediction program for predicting a fragment
20 structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step;

a prediction result comparison step that compares a fragment structure prediction result of the fragment structure prediction program
25 allowed to execute by the fragment structure prediction program

execution step with the tertiary structure data acquired by the tertiary structure data acquisition step;

a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein
5 based on a comparison result of the prediction result comparison step;
and

an interaction site prediction step that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

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12. The computer readable recording medium according to claim 10 or 11, further comprising:

a certainty factor information setting step that sets certainty factor information indicating a certainty factor for the fragment structure
15 prediction result of the fragment structure prediction program, wherein
the frustration calculation step calculates the frustration of the local part based on the certainty factor information set by the certainty factor information setting step and on the comparison result.

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